Journal of Molecular Spectroscopy

VOLUME 150, 1991

Editor
K. Narahari Rao

Editorial Committee

Frank C. De Lucia Jon T. Hougen James K. G. Watson

ACADEMIC PRESS, INC.
Harcourt Brace Jovanovich, Publishers
San Diego New York Boston
London Sydney Tokyo Toronto

Copyright © 1991 by Academic Press, Inc.

ALL RIGHTS RESERVED

No part of this publication may be reproduced or transmitted in any form or by any means, electronic or mechanical, including photocopy, recording, or any information storage and retrieval system, without permission in writing from the copyright owner.

The appearance of the code at the bottom of the first page of an article in this journal indicates the copyright owner's consent that copies of the article may be made for personal or internal use, or for the personal or internal use of specific clients. This consent is given on the condition, however, that the copier pay the stated per copy fee through the Copyright Clearance Center, Inc. (27 Congress Street, Salem, Massachusetts 01970), for copying beyond that permitted by Sections 107 or 108 of the U. S. Copyright Law. This consent does not extend to other kinds of copying, such as copying for general distribution, for advertising or promotional purposes, for creating new collective works, or for resale. Copy fees for pre-1991 articles are as shown on the article title pages; if no fee code appears, the copy fee is the same as for current articles.

0022-2852/91 $3.00

MADE IN THE UNITED STATES OF AMERICA

CONTENTS OF VOLUME 150

NUMBER 1, NOVEMBER 1991

JOHN A. COXON AND PHOTOS G. HAJIGEORGIOU. Isotopic Dependence of Born–Oppenheimer Breakdown Effects in Diatomic Hydrides: The $X^1\Sigma^+$ States of HI/DI and HBr/DBr 1

W. HÖHE AND W. A. KREINER. $K = 3$ Splitting and Quadrupole Hyperfine Structure in the ν_1 Fundamental of Nitrogen Trifluoride 28

JOHN A. COXON, MINGGUANG LI, AND PAUL I. PRESUNKA. Laser Fluorescence Excitation Spectroscopy of CaOH and CaOD: The $A^2\Pi$–$X^2\Sigma^+$ (100)–(000) Band System and the (100)–(020) Fermi Resonance 33

PAULO J. A. RIBEIRO-CLARO, JOSÉ J. C. TEIXEIRA-DIAS, ROBERT D. GORDON, AND J. MICHAEL HOLLAS. Vibration Wavenumbers of 3-Aminobenzotrifluoride in the Ground and S_1 Electronic States from Its Infrared, Raman, and Supersonic Jet S_1–S_0 Fluorescence Spectra 46

MILJENKO PERIĆ, BERND ENGELS, AND SIGRID D. PEYERIMHOFF. Ab Initio Investigation of the Vibronic Structure of the C_2H Spectrum: Calculation of the Hyperfine Coupling Constants for the Three Lowest-Lying Electronic States 56

MILJENKO PERIĆ, BERND ENGELS, AND SIGRID D. PEYERIMHOFF. Ab Initio Investigation of the Vibronic Structure of the C_2H Spectrum: Computation of the Vibronically Averaged Values for the Hyperfine Coupling Constants 70

KENNETH G. UNFRIED AND R. F. CURL. Infrared Flash Kinetic Spectroscopy of ν_2 of Ketenyl Radical 86

J. BEHREND, P. MITTLER, G. WINNEWISSER, AND K. M. T. YAMADA. Spectra of Deuterated Disulfane and Spectroscopic Determination of Its Molecular Structure 99

M. W. EVANS. Optical NMR and ESR 120

PER JENSEN, I. PAIDAROVÁ, J. VOJTÍK, AND V. ŠPIRKO. Theoretical Calculations of the Nuclear Quadrupole Coupling in the Spectra of D_3^+, H_2D^+, and HD_2^+ 137

DANIEL LAMBOT, GHISLAIN BLANQUET, JACQUES WALRAND, AND JEAN-PIERRE BOUANICH. Diode-Laser Measurements of H_2-Broadening Coefficients in the ν_5 Band of C_2H_2 164

CURTIS P. RINSLAND, MARY ANN H. SMITH, V. MALATHY DEVI, AND D. CHRIS BENNER. Measurements of Lorentz-Broadening Coefficients and Pressure-Induced Line Shift Coefficients in the ν_2 Band of $D_2{}^{16}O$ 173

S. GIORGIANNI, P. STOPPA, A. BALDACCI, A. GAMBI, AND S. GHERSETTI. Diode Laser Measurements of CF_3Cl near 1258 cm^{-1}: Rovibrational Analysis of $\nu_2 + \nu_3$ Combination and Its Hot Bands 184

WILLIAM E. JONES AND THOMAS D. MCLEAN. Spectroscopic Investigation of InCl in the Ultraviolet: The $C^1\Pi$–$X^1\Sigma$ System 195

J. M. JOUVARD, B. LAVOREL, J. P. CHAMPION, AND L. R. BROWN. Preliminary Analysis of the Pentad of $^{13}CH_4$ from Raman and Infrared Spectra 201

HENDRIK F. HAMEKA, JAMES O. JENSEN, JACK G. KAY, CAREY M. ROSENTHAL, AND GEORGE L. ZIMMERMAN. Theoretical Prediction of Geometries and Vibrational Infrared Spectra of Ruthenium Oxide Molecules 218
E. CANÉ, A. TROMBETTI, B. VELINO, AND W. CAMINATI. Assignment of the 278-nm Electronic Band System of Benzimidazole [1,3-Benzodiazole] as $\pi^*-\pi$ by Rotational Band Contour Analysis 222
ROLF MEYER AND WALTHER CAMINATI. Quartic Centrifugal Distortion Constants Derived from a Flexible Model for 3-Methylthietan 229
NOBUKIMI OHASHI AND MASATO MASUE. Explicit Expressions for Torsional–Wagging–Rotational Hamiltonian Matrix Elements in Hydrazine-like Molecules 238
A. BARBE, S. BOUAZZA, J. J. PLATEAUX, J. M. FLAUD, AND C. CAMY-PEYRET. Line Positions and Intensities of the $2\nu_3$, $\nu_1 + \nu_3$, and $2\nu_1$ Bands of $^{18}O_3$ 255
TAKASHI ISHIWATA, OSAMU NAKAMURA, AND KINICHI OBI. Optical–Optical Double Resonance Spectroscopy of the Br_2 $0_g^+(^1D)$ Ion-Pair State 262
M. BENAVIDES-GARCIA AND K. BALASUBRAMANIAN. Spectroscopic Constants and Potential Energy Curves for OsH 271

NOTES

M. FEHÉR, C. SALUD, J. P. MAIER, AND A. J. MERER. On the *J*-Assignment of the Infrared Laser Spectrum of CCN 280
MAREK RYTEL AND TERESA RYTEL. The Application of Jackiw's Sum Rules to Radial Problems 282
A. S-C. CHEUNG, J. P. L. LI, T. W. WONG, MINGGUANG LI, AND H. E. RADFORD. Far-Infrared Laser Magnetic Resonance Spectrum of SO in the $X^3\Sigma^-$ State 285
T. PRADEEP, M. S. HEGDE, AND C. N. R. RAO. An Ultraviolet Photoelectron Spectroscopic Study of the Hydrogen Bonded Dimers of Methanol, Ethanol, and Dimethylamine in the Vapor Phase 289
M. HERMAN, D. HURTMANS, J. VANDER AUWERA, AND M. VERVLOET. Lack of Intensity Alternation in C_2H_2 293
DANIEL C. ROBIE, JULIAN DE JUAN, AND HANNA REISLER. Assignment of the 278.2-nm Peak of the CCl $A^2\Delta$–$X^2\Pi$ System as the 0–0 P_1 Bandhead 296

ANNOUNCEMENTS 300

NUMBER 2, DECEMBER 1991

DAVID S. GREEN, GRANT A. BICKEL, AND STEPHEN C. WALLACE. (2 + 1) Resonance Enhanced Multiphoton Ionization of Hydrogen Chloride in a Pulsed Supersonic Jet: Spectroscopic Survey 303
DAVID S. GREEN, GRANT A. BICKEL, AND STEPHEN C. WALLACE. (2 + 1) Resonance Enhanced Multiphoton Ionization of Hydrogen Chloride in a Pulsed Supersonic Jet: Spectroscopy and Rydberg ~ Valence Interactions of the $^1\Sigma^+(0^+)$ and $^3\Sigma^-(1, 0^+)$ States 354

DAVID S. GREEN, GRANT A. BICKEL, AND STEPHEN C. WALLACE. (2 + 1) Resonance Enhanced Multiphoton Ionization of Hydrogen Chloride in a Pulsed Supersonic Jet: Vacuum Wavenumbers of Rotational Lines with Detailed Band Analysis for Excited Electronic States of $H^{35}Cl$ 388

WEIDONG CHEN, R. BOCQUET, D. BOUCHER, J. DEMAISON, AND G. WLODARCZAK. The Submillimeterwave Rotational Spectra of CH_3CN and CD_3CN. Analysis of the $v_8 = 1$ and $v_8 = 2$ Excited Vibrational States ... 470

E. MAHIEU, I. DUBOIS, AND H. BREDOHL. Rotational Analysis of the $a^3\Pi_r$–$X^1\Sigma^+$ Transition of $^{69}Ga^{35}Cl$ 477

T. L. TAN, E. C. LOOI, K. T. LUA, A. G. MAKI, J. W. C. JOHNS, AND M. NOËL. Infrared Spectrum of the ν_9 and $2\nu_9$–ν_9 Bands of Deuterated Nitric Acid (DNO_3) 486

M. LE GUENNEC, W. CHEN, G. WLODARCZAK, J. DEMAISON, R. EUJEN, AND H. BÜRGER. The Millimeterwave Spectrum of Germyl Fluoride: Determination and Comparison of the Effective, Substitution, and Equilibrium Structures 493

V. C. EPA AND P. R. BUNKER. The Watson $U(\rho)$ Term in the One-Dimensional Semirigid Bender Hamiltonian for the HF Dimer 511

P. LIU, J. KIECKHÄFER, AND E. TIEMANN. Hyperfine Structure in the $B^3\Pi_{0+u}$ State of Br_2 and the Influence of the Perturbing 1_u State 521

D. D. NELSON, JR., AND M. S. ZAHNISER. Diode Laser Spectroscopy of the ν_3 Vibration of the HO_2 Radical 527

Y. KABBADJ, M. HERMAN, G. DI LONARDO, L. FUSINA, AND J. W. C. JOHNS. The Bending Energy Levels of C_2H_2 535

C. I. FRUM, R. ENGLEMAN, JR., AND P. F. BERNATH. Fourier Transform Emission Spectroscopy of the $A'^3\Pi$–$X^3\Sigma^-$ Transition of PtO 566

K. MATSUMURA, F. J. LOVAS, AND R. D. SUENRAM. Fourier-Transform Microwave Spectroscopy of the Deuterated Acetylene Dimers: The Interconversion Tunneling Motions of $(DCCD)_2$, $(DCCH)_2$, DCCD–DCCH, DCCH–DCCD, HCCH–DCCD, and HCCH–DCCH 576

JOHN A. FERNLEY, STEVEN MILLER, AND JONATHAN TENNYSON. Band Origins for Water up to 22 000 cm^{-1}: A Comparison of Spectroscopically Determined Potential Energy Surfaces 597

HARUKI ISHIKAWA AND OKITSUGU KAJIMOTO. Fermi Resonance and Vibrational Analysis of SiH_2 ($\tilde{X}^1A_1$) Based on the LIF Excitation Spectra of the $\tilde{A}^1B_1$ (060) ← $\tilde{X}^1A_1$ ($0v''0$) Transitions 610

D. MCNAUGHTON AND D. N. BRUGET. The High-Resolution Infrared Spectrum of Triacetylene 620

NOTES

D. MCNAUGHTON AND E. G. ROBERTSON. The Microwave Spectrum of 3,4-Pyridinedicarboxylic Anhydride 635

CURTIS P. RINSLAND, MARY ANN H. SMITH, V. MALATHY DEVI, AND D. CHRIS BENNER. Measurements of Lorentz-Broadening Coefficients and Pressure-Induced Line Shift Coefficients in the ν_2 Band of $HD^{16}O$ 640

LETTER TO THE EDITOR

RANDY D. MAY AND DEAN B. PETERSON. Observation of the O–O Stretch Fundamental Band of HO_2NO_2 647

AUTHOR INDEX FOR VOLUME 150 650

SUBJECT INDEX FOR VOLUME 150 652